Nitrofurantoin 67-20-9 | DTXSID7020972

Model Performance

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N	Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (75	Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: -0.793

Global applicability domain: Inside

Local applicability domain index: 4.32e-01

Confidence level: 3.89e-01

Nearest Neighbors from the Training Set

Image not found

Nitrofurantoin

Measured: -0.470 Predicted: -0.793

Image not found

Furazolidone

Measured: -0.0400 Predicted: 5.28e-01 Image not found

N-Pyrazin-2-ylalanine Measured: -2.79 Predicted: 3.87e-01